

Fluid dynamics parameters of a high temperature ejector for SOFC anode gas recirculation

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Abstract. The energy sector embraces solid oxide fuel cells (SOFC) since they are highly efficient and ecologically sound power generators. Yet, maintaining fuel cells sustainability in power units takes a lot of resources. Hence, we need to find the appropriate ways to increase the efficiency of the whole SOFC power system inclusive of its balance-of-plant equipment. This can facilitate our fuel and energy complex green transition through the SOFC technology introduction. As a matter of fact, anode gas recirculation is instrumental for boosting the SOFC power units efficiency. One of the challenges in developing the SOFC power unit with anode gas recirculation is to return the amount of anode gas appropriate for carbon deposition free reforming. The paper contains the anode gas recirculation ratio in the SOFC power units calculation method for various reforming temperatures. The safest operation modes of the SOFC power units with anode gas recirculation were determined. The 3 kW SOFC power unit with high temperature ejector and nickel-based catalyst for methane conversion was designed. For the given flow channel geometry, the high temperature ejector off-design performance was plotted. In addition, fields of temperature, pressure and velocities were plotted for the ejector design point using Ansys computational fluid dynamics software.

1. Introduction

Fuel cells allow direct conversion of chemical energy of fuel into electricity. For small distributed energy solid oxide fuel cells (SOFC) are the most attractive since air and synthesis gas can be used as an oxidizing agent and fuel respectively while other solutions may require pure oxygen and hydrogen for operation. Working at high temperature (750-1000°C) the SOFC need no precious metal catalysts.

The most common scheme of SOFC power unit includes steam reforming of natural gas. The efficiency of the scheme may reach 70%, but its implementation requires a source of water and heat for endothermic steam reforming reaction occurring. Such features fail to allow a wide use of this scheme for the supply of autonomous and remote objects. In this case, it is possible to apply the scheme with the methane partial oxidation by air oxygen. This scheme has a considerably lower efficiency than the steam reforming solution, but the reformer is more compact and there is no need in water source and the reformer heating, which certainly improves the independence of the equipment [1]. The most promising SOFC power unit scheme involves anode gas recirculation since it is as independent as the air reforming solution and has efficiency comparable to the steam reforming. In this scheme one part of the anode off gas is reinjected into the reformer where steam and dry reforming reactions take place [2, 3].

A major challenge when implementing the anode off-gases recirculation is to ensure effective return of the sufficient amount of the gases to maintain the reforming reactions and avoid carbon deposition.



There are a number of publications devoted to the SOFC anodic recirculation systems in which the recirculation is achieved by ejectors or blowers [4–12]. Halinen et al. [10] due to unreliability of ejector transient operation and complexity in its manufacture have decided to implement the recirculation with a blower. However, the blowers decrease the system efficiency as they consume electricity. Moreover, significant changes must be made to integrate the blower in the existing schemas and there is also a risk of oil and grease leakage into the recirculated gases which may adversely affect the reformer catalyst and the fuel cells anodes [11]. The researchers [7–9, 11] used various designs of ejectors to return anode off-gases at nominal operation mode. For variable-load operation modes D. A. Brunner et al. [12] have proposed a variable flow ejector with a needle for changing the primary nozzle cross section to accommodate the system load changes. This needle is actuated by an engine. Therefore, the solution has moving parts and consumes electrical energy which reduce the system reliability and efficiency. In this paper, the ejector design for the SOFC systems with anode off-gases recirculation and its control method based on the primary flow temperature changing are presented.

2. Modeling SOFC power unit with anode off-gases recirculation

The SOFC power unit with anode off-gases recirculation differs from the schemes with air and steam reforming of natural gas by the presence of the mixing device (ejector) and the absence of need in supplying an external flow to the reformer besides natural gas. The greatest challenge in this scheme is the carbon deposition prevention in the reformer and the SOFC stacks in some operation modes. In order to avoid carbon deposition it is necessary to determine the anode off-gases recirculation ratio at different SOFC temperatures and fuel utilization rates.

2.1. SOFC power unit with anode off-gases recirculation layout

Figure 1 shows a layout of the SOFC power unit with anode off-gases recirculation. Natural gas at a pressure of 2 bar (absolute) is supplied to the ejector as a primary flow entraining a part of the anode off-gases (secondary flow) at a pressure of 1 bar (absolute) equal to the recirculation ratio z . The resulting mixture of gases at a greater pressure in relation to the secondary flow is fed to the reformer with a nickel-based catalyst where it is converted to the synthesis gas in steam and dry reforming. The synthesis gas derived is then supplied to the SOFC anode, where its combustible components are oxidized by oxygen ions diffusing through the solid electrolyte from the cathode channel. This electrochemical reaction produces electric current and makes the anode off-gases depleted in hydrogen and enriched in water vapor.

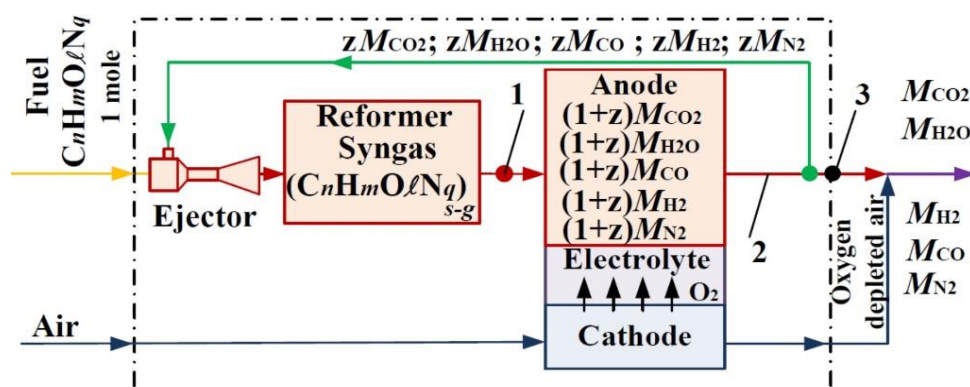


Figure 1. The SOFC power unit with recirculation layout. 1 – fuel utilization rate at the reformer outlet, $\alpha_{ref,out}$; 2 – fuel utilization rate at the SOFC stack outlet downstream the reformer, $\alpha_{sofc,out}$; 3 – fuel utilization rate at the SOFC stack outlet upstream the reformer, $\alpha_{f,out}$.

2.2. Method of calculating recirculation ratio z at which the carbon deposition fails to occur in the reformer and fuel cell anode channel

The following nonlinear equations set based on component balance equations and equilibrium constant expressions for reforming reactions can be used for finding the minimum recirculation ratio z_{min} ensuring carbon deposition free operation at given reformer temperature [13]:

$$M_{\text{CO}_2} + M_{\text{CO}} + M_{\text{CH}_4} = n(1+z), \quad (1)$$

$$2M_{\text{H}_2\text{O}} + 2M_{\text{H}_2} + 4M_{\text{CH}_4} = m(1+z), \quad (2)$$

$$2M_{\text{CO}_2} + M_{\text{CO}} + M_{\text{H}_2\text{O}} = l(1+z) + z\alpha_{\text{f,out}}(2n + 0.5m - l), \quad (3)$$

$$2M_{\text{N}_2} = q(1+z), \quad (4)$$

$$\frac{M_{\text{CO}_2} \cdot M_{\text{H}_2}}{M_{\text{CO}} \cdot M_{\text{H}_2\text{O}}} = K, \quad (5)$$

$$\frac{M_{\text{CO}} \cdot M_{\text{H}_2} \cdot p}{M_{\text{H}_2\text{O}} \cdot M_{\text{g}} \cdot a_{\text{c}}} = K_2. \quad (6)$$

where $M_{\text{CO}_2}, M_{\text{H}_2\text{O}}, M_{\text{CO}}, M_{\text{H}_2}, M_{\text{CH}_4}, M_{\text{N}_2}$ – molar quantities of gaseous reaction products and M_{g} is their sum; n, m, l, q – atomic ratios of carbon, hydrogen, oxygen and nitrogen in a molecule of fuel, respectively; p – absolute reformer pressure; K – shift reaction equilibrium constant; K_2 – shift reaction equilibrium constant; a_{c} – carbon activity ($a_{\text{c}} = 1$ as carbon is in the form of graphite).

In turn, z_{min} depends on the SOFC fuel utilization rate and the latter is smaller, the greater amount of anode off-gases must be returned to the reformer. The solution of the equations set (1)-(6) has shown that given the reformer temperature is above 1073 K (800 °C) the system operates without carbon deposition at $\alpha_{\text{f,out}} > 0.6$ and $z > 0.7$. Therefore it is necessary to maintain the appropriate values of $\alpha_{\text{f,out}}$ and z to ensure the reformer and SOFC stack safe operation.

In order to calculate the ejector entrainment ratio u the molar quantities of fuel and synthesis gas components were multiplied by the corresponding molar masses term by term. As a result, the apparent masses of primary and mixed flows were obtained. Further, applying the mass conservation equation to the ejector-reformer system the apparent mass of the secondary flow was obtained. Finally, the entrainment ratio is calculated as the proportion of the secondary flow compared to the primary flow masses. The calculation indicates that the entrainment ratio is ranging from 2.4 to 3.8 for carbon deposition free modes of operation at $0.6 < \alpha_{\text{f,out}} < 0.8$ and $0.7 < z < 0.9$ and it is independent of temperature given z and $\alpha_{\text{f,out}}$ are constant.

3. SOFC power unit with anode off-gases recirculation ejector design and control

Based on the above calculations, the ejector design was carried out for the following system parameters:

- net power, $N = 3$ kW; efficiency, $\eta = 0.4$; fuel: methane, $\rho = 0.714$ kg/m³;
- fuel flow rate $G_{\text{P}} = 14.93 \cdot 10^{-5}$ kg/s; SOFC fuel utilization rate, $\alpha_{\text{f,out}} = 0.7$;
- recirculation ratio $z = 0.8$; entrainment ratio $u = 3$;
- primary flow inlet temperature $T_{\text{P}} = 20$ °C; secondary flow inlet temperature $T_{\text{S}} = 800$ °C;
- primary flow inlet pressure $P_{\text{P}} = 2$ bar; secondary flow inlet pressure $P_{\text{S}} = 1$ bar;
- anode off-gas composition: $\text{CO}_2 = 20.5\%$; $\text{H}_2\text{O} = 39.6\%$; $\text{CO} = 12.8\%$; $\text{H}_2 = 27.1\%$; $\text{CH}_4 = 0\%$.

3.1. Ejector design

The main radial and axial dimensions of the ejector were defined and its design is shown in figure 2.

According to the [14], the nozzle throat cross section area $f_{\text{P}} = 4.32 \cdot 10^{-7}$ m², the mixing chamber is $f_{\text{M}} = 1.91 \cdot 10^{-5}$ m², distance from the nozzle outlet to the mixing chamber inlet is $L_{\text{PM}} = 6.4$ mm. The mixing chamber and diffuser lengths were taken depending on the mixing chamber diameter: $L_{\text{M}} = 8.8 \cdot d_{\text{M}} = 44$ mm [14], $L_{\text{D}} = 6.8 \cdot d_{\text{M}} = 34$ mm [15] respectively. The angle employed in the junction of the suction and the mixing chamber is 45° [14], the convergent nozzle angle is 6° and the diffuser included angle is 4° [15].

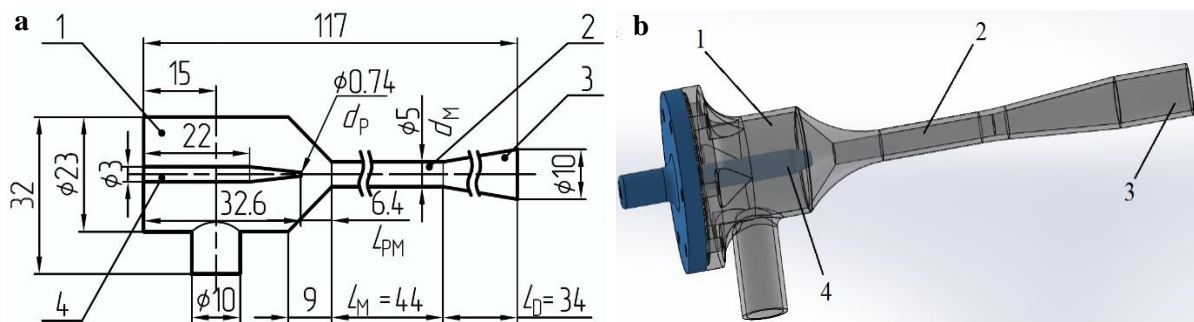


Figure 2. Ejector flow channel geometry (a) and 3D model (b). 1 – suction chamber; 2 – mixing chamber; 3 – diffuser; 4 – nozzle.

3.2. Ejector model validation

Before conducting experiments with natural gas the ejector will be tested with nitrogen and air. For this purpose, the ejector flow channel geometry performance was numerically and theoretically studied for both combustible and non-combustible gases. This was done in two ways. Firstly, the designed ejector performance was numerically modeled in Ansys Fluent [16]. Secondly, the ejector flow channel geometry was used for plotting its control characteristics map [14] as described in the next section.

The design point (fixed inlet temperatures and pressures) simulations for nitrogen/air using Ansys Fluent and the semiempirical model [14] show that the designed ejector performance is sustainable for non-combustible gases. Moreover, these two analysis methods correlate with each other, i.e. the mixed flow temperature obtained using the semiempirical model is 878 K and the Ansys Fluent yields 855 K (deviation from the semiempirical model is 2.6%). However, the key advantage of the CFD method is an opportunity to observe processes inside the ejector. As a result, fields of temperature, pressure and velocities were plotted for the ejector design point (figures 3-5). They are crucial for the ejector manufacture as they can be used to prevent thermal strains during hot tests and air infiltration.

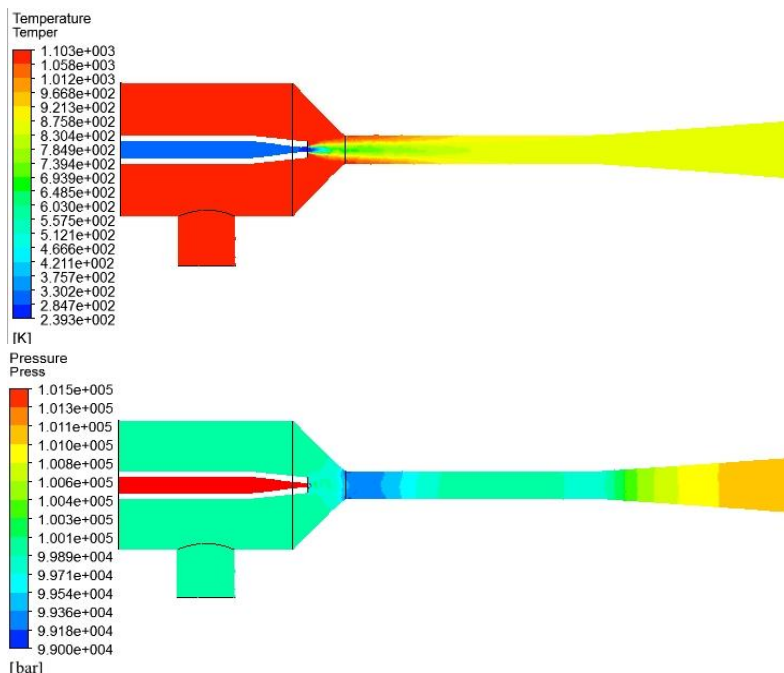


Figure 3. Field of temperature (Kelvin) in longitudinal section of the ejector flow channel.

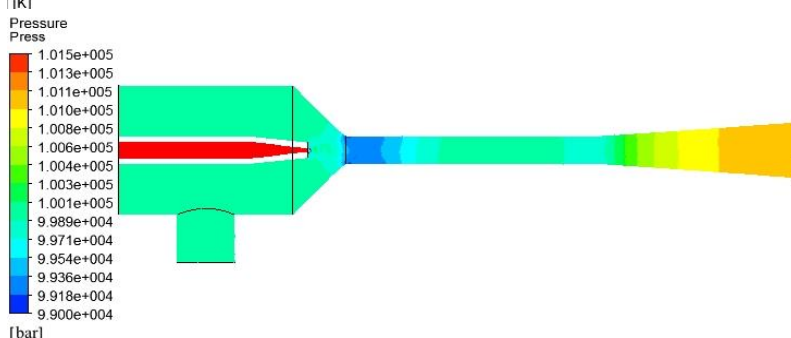


Figure 4. Field of pressure (bar) in longitudinal section of the ejector flow channel.

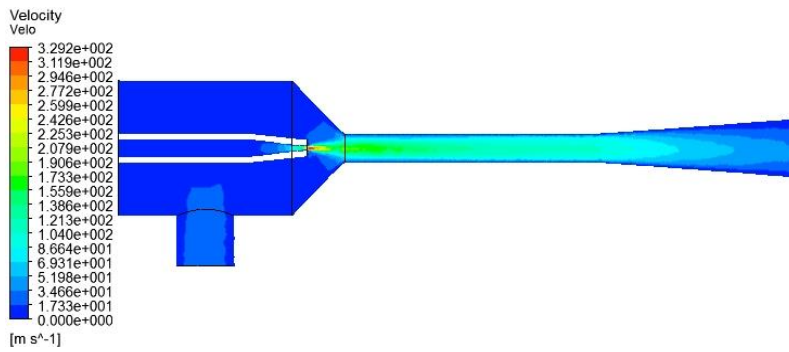


Figure 5. Field of velocities (m/s) in longitudinal section of the ejector flow channel.

3.3. SOFC anode gas recirculation control method

Employing the semiempirical model [14] we obtained the control characteristics map [14] for various media. The model accounts for losses due to the ejector flow channel geometry. Given the SOFC unit net power output decreases from 3 kW to 2 kW, the natural gas mass flow rate through the nozzle is to be decreased from $14.93 \cdot 10^{-5}$ kg/s to $9.95 \cdot 10^{-5}$ kg/s without the mixed flow pressure drop. The entrainment ratio is also to be kept in the range from 2.4 to 3.8 to avoid carbon deposition. The ejector flow channel geometry being fixed, it can be carried out by either primary flow pressure decrease or temperature increase according to the equation:

$$G_P = \rho_P f_P \sqrt{k_P R_P T_P} \left(\frac{2}{k_P + 1} \right)^{\frac{k_P + 1}{2(k_P - 1)}}, \quad (7)$$

where R – gas constant, J/kg·K; ρ – density, kg/m³.

The ejector control characteristics map is shown in figure 6. It follows that the designed ejector can operate on both combustible and non-combustible gases. This map also gives a path to create the suitable SOFC anode gas recirculation control method. The design points are A_1 and A_2 for both combustible and non-combustible gases respectively. If the primary mass flow rate is decreased by its inlet pressure drop and the mixed flow pressure is constant, the entrainment ratio for these off-design conditions is lower than 2.4 (points B_1 and B_2) which can cause the SOFC power unit to malfunction. However, if the ejector is controlled by changing the primary flow inlet temperature, the unit performance is more sustainable as the mixed flow pressure rises at the constant entrainment ratio (points C_1 and C_2).

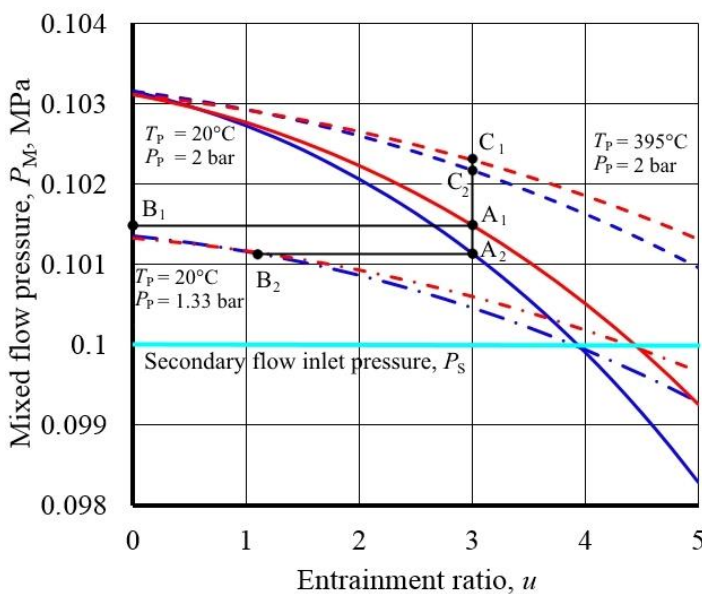


Figure 6. The ejector control characteristics map. Red – combustible gases; dark blue – non-combustible gases. Solid line – design point inlet temperature and pressure; dash-dot line – primary flow pressure is 1.33 bar; dash line – primary flow temperature is 395 °C.

4. Conclusions

The anode gas minimum recirculation ratio ensuring carbon deposition free operation of the SOFC power units calculation method showed that the entrainment ratio is ranging from 2.4 to 3.8 for carbon deposition free modes of operation at $0.6 < \alpha_{f,out} < 0.8$ and $0.7 < z < 0.9$.

Based on the obtained data, the ejector design was carried out and its functional prototype was produced for the 3 kW SOFC power unit. The ejector testing was planned and its control method based on the primary flow temperature changing was presented.

The ejector CFD simulation in Ansys Fluent was compared with its semiempirical modelling according to [14]. Deviation from the semiempirical model was 2.6% which is enough for the CFD analysis validation.

The control characteristics map and fields of temperature, pressure and velocities for the SOFC power unit with anode gas recirculation ejector design point will be used in further studies.

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